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MAGNETIC PROPERTIES OF TITANIUM CARBIDE (TIC) DIATOMIC MOLECULE UNDER THE INFLUENCE OF MAGNETIC AND AHARONOV–BOHM FLUX FIELDS AT FINITE TEMPERATURE

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ABSTRACT

In this study, the influence of magnetic and Aharonov–Bohm (AB) flux fields on the magnetic properties of the Titanium Carbide (TiC) diatomic molecule at finite temperature is investigated. Using the generalized cosine Yukawa potential within the framework of the Nikiforov–Uvarov Functional Analysis (NUFA) method, the energy eigenvalue and the corresponding energy eigenfunction as well as the partition functions were obtained. Based on these, temperature-dependent magnetization, magnetic susceptibility, and persistent current were evaluated. The results show that magnetization increases with both magnetic field strength and AB flux, but decreases with temperature due to enhanced thermal agitation that disrupts magnetic dipole alignment. Similarly, magnetic susceptibility and persistent current diminish with temperature but exhibit higher magnitudes at stronger field intensities. These behaviors are consistent with Curie-like paramagnetism and agree with previous findings on related diatomic systems.

1 INTRODUCTION

In quantum mechanics, the Schrödinger Equation (SE) serves as a fundamental second-order differential equation that characterizes the behavior of non-relativistic system [1]. Over time, various analytical methods have been developed to solve the SE for different physical systems. These approaches include the supersymmetric quantum mechanics (SUSYQM) method [2], Nikiforov–Uvarov (NU) method [3], formula method [4], ansatz method [5], Qiang–Dong proper quantization rule [6, 7], factorization method [8] among others. These techniques have been extensively applied to obtain solutions for the SE with various potentials [9-14] including central and non-central potentials, in both bound and scattering state problems.

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Exponential Coulomb (EC) potentials, with or without cosine terms, are particularly significant in fields like plasma physics, nuclear physics, condensed matter physics, and atomic physics [15-20]. The EC potential, also known as the Screened Coulomb (SC) potential, is expressed as:

$$V(r) = -\frac{A}{r}e^{-\alpha r} \qquad (1)$$

where α is the screening parameter and A is strength coupling constant. In recent years, researchers have focused on solving the Schrödinger equation (SE) under the influence of magnetic and Aharonov–Bohm (AB) flux fields in two-dimensional spaces, as demonstrated by [21]. Ikhdair and Hamzavi [22] examined the eigensolutions for charged particles confined by harmonic oscillators subjected to strong magnetic and AB flux fields, revealing notable modifications in the spectral properties. The Dirac equation has also been employed to explore spin and pseudospin symmetries in quantum systems influenced by external electromagnetic fields. Additionally, the Killingbeck potential was analyzed under similar field conditions using power-series techniques by Hamzavi, Ikhdair & Thylwe [23] and Kumar & Chand [24]. Collectively, these investigations have significantly advanced the understanding of quantum systems under the effect of magnetic and AB flux fields [25, 26]. To the best of our knowledge, no previous study has examined the influence of magnetic and AB flux fields on the magnetic properties of the TiC diatomic molecule with generalized cosine Yukawa potential. In response to this gap, the aim of this paper is to investigate these effects using the generalized cosine Yukawa potential [27] within the NUFA [28] method. The study specifically addresses the following research questions: How does the magnetic field strength (B) influence the magnetization of the TiC diatomic molecule at finite temperatures? What is the effect of the Aharonov–Bohm (AB) flux field (Φ_{AB}) on the magnetization behavior of the TiC diatomic molecule? How do temperature variations (through inverse temperature $\beta = 1/k_B T$) affect the magnetization, magnetic susceptibility and persistent current of the TiC diatomic molecule? What is the combined influence of magnetic and AB flux fields on the magnetic susceptibility and persistent current of TiC? Are the observed magnetic responses of TiC consistent with previously reported behaviors in similar diatomic systems, such as TiH? The potential model [29] adopted for this study is given as:

$$V(r) = -2D_e\frac{A}{\eta}e^{-\xi\eta}\cosh(\xi\eta) \qquad (3)$$

or explicitly

$$V(r) = -D_e\frac{A}{\eta}\left(1+e^{-2\xi\eta}\right) \qquad (4)$$

where D_e denotes dissociation energy, $A \equiv \eta_e$ denotes equilibrium bond length, ξ denotes screening parameter.

2. Nikiforov-Uvarov Functional Analysis (NUFA) Method

In this section, we briefly introduce Nikiforov-Uvarov Functional Analysis (NUFA) method [28]. This method is useful to solve second-order differential equation wave equations of the hypergeometry-type:

$$\frac{d^2\psi(s)}{ds^2} + \frac{\tilde{\tau}(s)}{\sigma(s)}\frac{d\psi(s)}{ds} + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0 \qquad (5)$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials at most second degree, and $\tilde{\tau}(s)$, is a first degree polynomial. The parametric form of NU method is in the form:

$$\frac{d^2\psi(s)}{ds^2}+\frac{\alpha_1-\alpha_2 s}{s(1-\alpha_3 s)}\frac{d\psi(s)}{ds}+\frac{1}{s^2(1-\alpha_3 s)^2}\left[-\xi_1 s^2+\xi_2 s-\xi_3\right]\psi(s)=0 \qquad (6)$$

where α_i and $\xi_i\,(i=1,2,3)$ are all paramters. It can be observed in Eq. (6) that the differential equation has two singularities at $s\to 0$ and $s\to 1$, thus it takes the wave function in the form

$$\psi(s)=s^{\lambda}(1-s)^{v}\,f(s) \qquad (7)$$

Substituting Eq. (7) into Eq. (6) leads to the following equation

$$s(1-\alpha_3 s)\frac{d^2 f(s)}{ds^2}+\left[\sigma_1+2\lambda-(2\lambda\alpha_3+2v\alpha_3+\alpha_2)s\right]\frac{df(s)}{ds}$$
$$-\alpha_3\left(\lambda+v+\frac{1}{2}\left(\frac{\alpha_2}{\alpha_3}-1\right)+\sqrt{\frac{1}{4}\left(\frac{\alpha_2}{\alpha_3}-1\right)^2+\frac{\xi_1}{\alpha_3^2}}\right)\left(\lambda+v+\frac{1}{2}\left(\frac{\alpha_2}{\alpha_3}-1\right)-\sqrt{\frac{1}{4}\left(\frac{\alpha_2}{\alpha_3}-1\right)^2+\frac{\xi_1}{\alpha_3^2}}\right)$$
$$+\left[\frac{\lambda(\lambda-1)+\alpha_1\lambda-\xi_3}{s}+\frac{v(v-1)\alpha_3+\alpha_2 v-\alpha_1\alpha_3 v-\frac{\xi_1}{\alpha_3}+\xi_2-\xi_3\alpha_3}{(1-\alpha_3 s)}\right]f(s)=0 \qquad (8)$$

Eq. (8) can be reduced to a Gauss hypergeometric equation if and only if the following functions vanished

$$\lambda(\lambda-1)+\alpha_1\lambda-\xi_3=0 \qquad (9)$$

$$v(v-1)\alpha_3+\alpha_2 v-\alpha_1\alpha_3 v-\frac{\xi_1}{\alpha_3}+\xi_2-\xi_3\alpha_3=0 \qquad (10)$$

Thus, Eq. (8) now becomes

$$s(1-\alpha_3 s)\frac{d^2 f(s)}{ds^2}+\left[\sigma_1+2\lambda-(2\lambda\alpha_3+2v\alpha_3+\alpha_2)s\right]\frac{df(s)}{ds}$$
$$-\alpha_3\left(\lambda+v+\frac{1}{2}\left(\frac{\alpha_2}{\alpha_3}-1\right)+\sqrt{\frac{1}{4}\left(\frac{\alpha_2}{\alpha_3}-1\right)^2+\frac{\xi_1}{\alpha_3^2}}\right)$$
$$\times\left(\lambda+v+\frac{1}{2}\left(\frac{\alpha_2}{\alpha_3}-1\right)-\sqrt{\frac{1}{4}\left(\frac{\alpha_2}{\alpha_3}-1\right)^2+\frac{\xi_1}{\alpha_3^2}}\right)f(s)=0 \qquad (11)$$

Solving Eqs. (9) and (10) completely give

$$\lambda=\frac{1}{2}\left((1-\alpha_1)\pm\sqrt{(1-\alpha_1)^2+4\xi_3}\right) \qquad (12)$$

$$v=\frac{1}{2\alpha_3}\left((\alpha_3+\alpha_1\alpha_3-\alpha_2)\pm\sqrt{(\alpha_3+\alpha_1\alpha_3-\alpha_2)^2+4\left(\frac{\xi_1}{\alpha_3}+\alpha_3\xi_3-\xi_2\right)}\right) \qquad (13)$$

Eq. (11) is the hypergeometric equation type of the form

$$x(1-x)\frac{d^2 f(x)}{dx^2}+\left[c+(a+b+1)x\right]\frac{df(x)}{dx}-[ab]\,f(x)=0 \qquad (14)$$

where a, b, c are given as follows

$$a=\sqrt{\alpha_3}\left(\lambda+v+\frac{1}{2}\left(\frac{\alpha_2}{\alpha_3}-1\right)+\sqrt{\frac{1}{4}\left(\frac{\alpha_2}{\alpha_3}-1\right)^2+\frac{\xi_1}{\alpha_3^2}}\right) \qquad (15)$$

$$b=\sqrt{\alpha_3}\left(\lambda+v+\frac{1}{2}\left(\frac{\alpha_2}{\alpha_3}-1\right)-\sqrt{\frac{1}{4}\left(\frac{\alpha_2}{\alpha_3}-1\right)^2+\frac{\xi_1}{\alpha_3^2}}\right) \qquad (16)$$

$$c=\alpha_1+2\lambda \qquad (17)$$

Setting either a or b equal to a negative integer $-n,$ the hypergeometric function $f(s)$ turns to a polynomial of degree $n.$ Hence, the hypergeometric function $f(s)$ approaches finite in the following quantum condition i.e. $a=-n,$ where $n=0,1,2,3,.....n_{\max}$.
Using the above quantum condition,

$$\sqrt{\alpha_3}\left(\lambda+v+\frac{1}{2}\left(\frac{\alpha_2}{\alpha_3}-1\right)+\sqrt{\frac{1}{4}\left(\frac{\alpha_2}{\alpha_3}-1\right)^2+\frac{\xi_1}{\alpha_3^2}}\right)=-n \qquad (18)$$

$$\lambda+v+\frac{1}{2}\left(\frac{\alpha_2}{\alpha_3}-1\right)+\frac{n}{\sqrt{\alpha_3}}=-\sqrt{\frac{1}{4}\left(\frac{\alpha_2}{\alpha_3}-1\right)^2+\frac{\xi_1}{\alpha_3^2}} \qquad (19)$$

Squaring both sides of Eq. (19) and rearrainging, one obtains the energy eigenvalues for the NUFA method as

$$\lambda^2+2\lambda\left(v+\frac{1}{2}\left(\frac{\alpha_2}{\alpha_3}-1\right)+\frac{n}{\sqrt{\alpha_3}}\right)+\left(v+\frac{1}{2}\left(\frac{\alpha_2}{\alpha_3}-1\right)+\frac{n}{\sqrt{\alpha_3}}\right)^2-\frac{1}{4}\left(\frac{\alpha_2}{\alpha_3}-1\right)^2-\frac{\xi_1}{\alpha_3^2}=0 \qquad (20)$$

By substituting Eqs. (12) and (13) into Eq. (7), one obtains the corresponding wave equation for the NUFA method as

$$\psi(s)=\mathbb{N}s^{\frac{(1-\alpha_1)+\sqrt{(\alpha_1-1)^2+4\xi_3}}{2}}(1-\alpha_3 s)^{\frac{(\alpha_3+\alpha_1\alpha_3-\alpha_2)+\sqrt{(\alpha_3+\alpha_1\alpha_3-\alpha_2)^2+4\left(\frac{\xi_1}{\alpha_3}+\alpha_3\xi_3-\xi_2\right)}}{2\alpha_3}}\,{}_2F_1(a,b,c;s) \qquad (21)$$

where $\mathbb{N}$ is normalization constant.

3. Solution of the 2D Schrodinger Equation for TiC Diatomic Molecule with Generalized Cosine Yukawa Potential

The Generalized Cosine Yukawa Potential under the influence of magnetic and AB
flux fields with charged particles can be written in cylindrical coordinates as follows [30]:

$$\left(-i\hbar\vec{\nabla}-\frac{e}{c}\vec{A}\right)^2\psi(r,\phi,z)=2\mu\left[E_{nm}-V(r)\right]\psi(r,\phi,z) \qquad (22)$$

where $\hbar$ denotes reduced Planck constant, e denotes charge of the particle, μ denotes effective mass of the system, c denotes speed of light and E_{nm} denotes energy level. To indicate the magnetic field and the AB-flux field together, we express the vector potential $\vec{A}$ as a superposition of two terms as $\vec{A}=\vec{A}_1+\vec{A}_2$ having the azimuthal components and external magnetic field with $\vec{\nabla}\times\vec{A}_1=\vec{B}$ and $\vec{\nabla}\cdot\vec{A}_2=0,$ where $\vec{B}$ is the magnetic field. Then, we assume

$$\vec{A}_1=\frac{\vec{B}e^{-2\xi\eta}}{1-e^{-2\xi\eta}}\hat{\phi} \qquad (23)$$

To represent Φ_{AB} flux, we take

$$\vec{A}_2 = \frac{\Phi_{AB}}{2\pi\eta}\hat{\phi} = \frac{\rho}{2\pi\eta}\hat{\phi} \qquad (24)$$

Therefore, the total vector potential reads

$$\vec{A} = \left(\frac{\vec{B}e^{-2\xi\eta}}{1-e^{-2\xi\eta}} + \frac{\rho}{2\pi\eta}\right)\hat{\phi} \qquad (25)$$

To solve the stationary Schrodinger equation, we make ansatz

$$\psi(\eta,\phi) = (2\pi\eta)^{-1/2} e^{im\phi}\Im_{nm}(\eta) \qquad m \in \mathbb{Z} = 0, \pm1, \pm2, \ldots \qquad (26)$$

where m is the magnetic quantum number. Substituting Eqs. (4), (25) and (26) into Eq. (22) and using the approximation proposed by Greene and Aldrich [31] given as:

$$\frac{1}{r} \approx \frac{\xi}{1-e^{-\xi\eta}} \quad \text{and} \quad \frac{1}{r^2} \approx \frac{\xi^2}{(1-e^{-\xi\eta})^2} \qquad (27)$$

and carrying some algebraic expressions, we get a radial 2nd order-like Differential Equation (DE) given as follows:

$$\Im''_{nm}(\eta) + \left[\begin{array}{l} \dfrac{2\mu E_{nm}}{\hbar^2} + \dfrac{4\mu\xi D_e A}{\hbar^2\left(1-e^{-2\xi\eta}\right)}\left(1+e^{-2\xi\eta}\right) - \dfrac{4m\xi\kappa\vec{B}e^{-2\xi\eta}}{\hbar\left(1-e^{-2\xi\eta}\right)^2} \\ -\dfrac{\kappa^2\vec{B}^2e^{-4\xi\eta}}{\hbar^2\left(1-e^{-2\xi\eta}\right)^2} - \dfrac{2\xi\kappa^2\vec{B}\rho e^{-2\xi\eta}}{\hbar^2\left(1-e^{-2\xi\eta}\right)^2\pi} - \dfrac{\left[(m+\varepsilon)^2 - \frac{1}{4}\right]\xi^2}{\left(1-e^{-2\xi\eta}\right)^2} \end{array}\right]\Im_{nm}(\eta) = 0 \qquad (28)$$

where we have defined the following parameters as $\kappa = -\frac{e}{c}$, $\phi_0 = \frac{2\pi\hbar c}{e}$ and $\varepsilon = \frac{\Phi_{AB}}{\phi_0} = \frac{\rho}{\phi_0}$.

For Mathematical simplicity and convenience, we introduce the following dimensionless abbreviations: $-\varepsilon_{nm} = \frac{2\mu E_{nm}}{\hbar^2\xi^2}, \mathbb{R} = \frac{4\mu D_e A}{\hbar^2\xi}, \mathbb{Z} = \frac{4m\kappa\vec{B}}{\hbar\xi}, \mathbb{C} = \frac{\kappa^2\vec{B}^2}{\hbar^2\xi^2}, \mathbb{Q} = \frac{2\kappa^2\vec{B}\rho}{\hbar^2\xi\pi}, \mathbb{N} = (m+\varepsilon)^2 - \frac{1}{4}$ (29)

By substituting a new variable $s = e^{-\xi\eta}$ into Eq. (28), then we can simply write Eq. (28) in the s-coordinate as follows:

$$\frac{d^2\Im_{nm}(\eta)}{ds^2} + \frac{(1-s)}{s(1-s)}\frac{d\Im_{nm}(\eta)}{ds} + \frac{1}{s^2(1-s)^2}\left[\begin{array}{l} -\left(\varepsilon_{nm} + \mathbb{R} + \mathbb{C}\right)s^2 + \left(2\varepsilon_{nm} - \mathbb{Z} - \mathbb{Q}\right)s \\ -\left(\varepsilon_{nm} - \mathbb{R} + \mathbb{N}\right) \end{array}\right]\Im_{nm}(\eta) = 0 \qquad (30)$$

By comparing Eq. (30) with the NUFA method of Eq. (6), we obtain the following

$$\alpha_1 = \alpha_2 = \alpha_3 = 1, \ \xi_1 = \varepsilon_{nm} + \mathbb{R} + \mathbb{C}, \ \xi_2 = 2\varepsilon_{nm} - \mathbb{Z} - \mathbb{Q}, \ \xi_3 = \varepsilon_{nm} - \mathbb{R} + \mathbb{N}, \ \lambda = \sqrt{\varepsilon_{nm} - \mathbb{R} + \mathbb{N}}$$

and $v = \frac{1}{2} + \sqrt{\mathbb{C} + \mathbb{N} + \mathbb{Z} + \mathbb{Q} + \frac{1}{4}}$ (31)

with Eq. (31), the energy eigenvalue of the Generalized Cosine Yukawa Potential under the influence of external magnetic and AB-flux fields is now deduced as:

$$\varepsilon_{nm} - \mathbb{R} + \mathbb{N} + 2\sqrt{\varepsilon_{nm} - \mathbb{R} + \mathbb{N}}\,(n+v) + (n+v)^2 - \left(\varepsilon_{nm} + \mathbb{R} + \mathbb{C}\right) = 0 \qquad (32)$$

Substituting Eqs. (28) into Eq. (32), we obtain

$$E_{nm}=\frac{\hbar^2\xi^2}{2\mu}\left[(m+\varepsilon)^2-\frac{1}{4}\right]-2\xi D_eA-\frac{\hbar^2\xi^2}{2\mu}\left[\frac{\frac{8\mu D_eA}{\hbar^2\xi}+\frac{\kappa^2\vec{B}^2}{\hbar^2\xi^2}-\left[(m+\varepsilon)^2-\frac{1}{4}\right]-(n+\Lambda)^2}{2(n+\Lambda)}\right]^2 \quad (33)$$

where $\Lambda=\frac{1}{2}+\sqrt{(m+\varepsilon)^2+\frac{\kappa^2\vec{B}^2}{\hbar^2\xi^2}+\frac{4m\kappa\vec{B}}{\hbar\xi}+\frac{2\kappa^2\vec{B}\rho}{\hbar^2\xi\pi}}$, $m=\pm1,\pm2,\pm3,...,$ and m is the magnetic quantum number. By substituting Eq. (29) and Eq. (31) into Eq. (7), we obtain the corresponding wave function for the NUFA method as:

$$\psi(s)=Ns^{\sqrt{\varepsilon_{nm}-\mathbb{R}+\mathbb{N}}}(1-s)^{\frac{1}{2}+\sqrt{\mathbb{C}+\mathbb{N}+\mathbb{Z}+\mathbb{Q}+\frac{1}{4}}}\,{}_2F_1(a,b,c;s) \quad (34)$$

where N_{nm} is normalization constant.

${}_2F_1\left(\lambda+v+\sqrt{\varepsilon_{nm}+\mathbb{R}+\mathbb{C}},\lambda+v-\sqrt{\varepsilon_{nm}+\mathbb{R}+\mathbb{C}},2\lambda+1;s\right)$ is the hypergeometric function.

The 3D nonrelativistic energy solutions of Eq. (33) is obtain by setting $m=\ell+\frac{1}{2}$

$$E_{nm}=\frac{\hbar^2\xi^2\ell(\ell+1)}{2\mu}-2\xi D_eA-\frac{\hbar^2\xi^2}{2\mu}\left[\frac{\frac{8\mu D_eA}{\hbar^2\xi}-\ell(\ell+1)-\left(n+\frac{1}{2}+\sqrt{\ell(\ell+1)+\frac{1}{4}}\right)^2}{2\left(n+\frac{1}{2}+\sqrt{\ell(\ell+1)+\frac{1}{4}}\right)}\right]^2 \quad (35)$$

where ℓ is the rotational quantum number.

4. Magnetic Properties of the Generalized Cosine Yukawa Potential for TiC Diatomic Molecule

Since Eq. (33) is obtained, we can proceed to obtain the partition function and other magnetic properties of (GCYP) for TiC molecule. The partition function $Z(\beta)$ at finite temperature T is obtained using the Boltzmann constant factor as [32]:

$$Z(\beta)=\sum_{n=0}^{\aleph}e^{-\beta E_{nm}} \quad (36)$$

where $\beta=\frac{1}{kT}$ and k is Boltzmann constant.

Substituting Eq. (33) into Eq. (36), we have:

$$Z(\beta)=\sum_{n=0}^{\aleph}e^{-\beta\left(\gamma-\lambda\left(\frac{\Omega-(n+\Lambda)^2}{2(n+\Lambda)}\right)^2\right)} \quad (37)$$

where n is the vibrational quantum number, $n=0,1,2,3,...,\aleph,$ $\aleph$ signifies the upper bound vibrational quantum number. For simplification and convinience, we have introduced the following notations:

$$\gamma=\frac{\hbar^2\xi^2}{2\mu}\left[(m+\varepsilon)^2-\frac{1}{4}\right]-2\xi D_eA,\lambda=\frac{\hbar^2\xi^2}{2\mu},\Omega=\frac{8\mu D_eA}{\hbar^2\xi}+\frac{\kappa^2\vec{B}^2}{\hbar^2\xi^2}-\left[(m+\varepsilon)^2-\frac{1}{4}\right] \quad (38)$$

The maximum value $n_{\max}$ can be obtain by setting $dE_{nm}/dn=0,$

$$n_{\max} = -\Lambda \pm \sqrt{\Omega} \tag{39}$$

Replacing the summation in Eq. (37) by an integral, we have:

$$Z(\beta) = \int_{0}^{\aleph} e^{-\beta\left(\gamma - \lambda\left(\frac{\Omega - (n+\Lambda)^2}{2(n+\Lambda)}\right)^2\right)} dn \tag{40}$$

If we set $\rho = n + \Lambda,$ we can re-write the above integral in the form:

$$Z(\beta) = \int_{\Lambda}^{\aleph+\Lambda} e^{\beta\left(\frac{Q_1}{\rho^2} + Q_2\rho^2 - Q_3\right)} d\rho \tag{41}$$

On evaluating the integral in Eq. (41), we obtain the partition function of the GCYP for TiC molecule in magnetic and AB-flux fields as follows:

$$Z(\beta) = \frac{e^{-2\sqrt{-\beta Q_1}\sqrt{-\beta Q_2} - \beta Q_3}\sqrt{\pi}\left(\begin{array}{l} Erf\left[\frac{\sqrt{-\beta Q_1}}{\Lambda} - \Lambda\sqrt{-\beta Q_2}\right] - e^{4\sqrt{-\beta Q_1}\sqrt{-\beta Q_2}} Erf\left[\frac{\sqrt{-\beta Q_1}}{\Lambda} + \Lambda\sqrt{-\beta Q_2}\right] \\ - Erf\left[\frac{\sqrt{-\beta Q_1}}{\Lambda + n_{\max}} - \Lambda\sqrt{-\beta Q_2} - n_{\max}\sqrt{-\beta Q_2}\right] + e^{4\sqrt{-\beta Q_1}\sqrt{-\beta Q_2}} Erf\left[\frac{\sqrt{-\beta Q_1}}{\Lambda + n_{\max}} + \Lambda\sqrt{-\beta Q_2} + n_{\max}\sqrt{-\beta Q_2}\right]\end{array}\right)}{4\sqrt{-\beta Q_2}} \tag{42}$$

From the obtained partition function of the given system, one can obtain magnetic properties such as magnetization at finite temperature $M(\beta)$, magnetic susceptibility at finite temperature $\chi_m(\beta)$ and persistent current at finite temperature $I(\beta)$ defined as follows [29]:

Magnetization at finite temperature is written as

$$M(\beta) = \frac{1}{\beta Z(\beta)} \frac{\partial Z(\beta)}{\partial \beta} \tag{43}$$

Magnetic susceptibility at finite temperature is written as

$$\chi_m(\beta) = \frac{\partial M(\beta)}{\partial \beta} \tag{44}$$

Persistent current at finite temperature is written as

$$I(\beta) = -\frac{e}{hc} \frac{\partial F(\beta)}{\partial \beta} \tag{45}$$

RESULTS

In this section, the graphical analysis for a TiC diatomic molecule is presented. The fitting parameters used are based on [33].

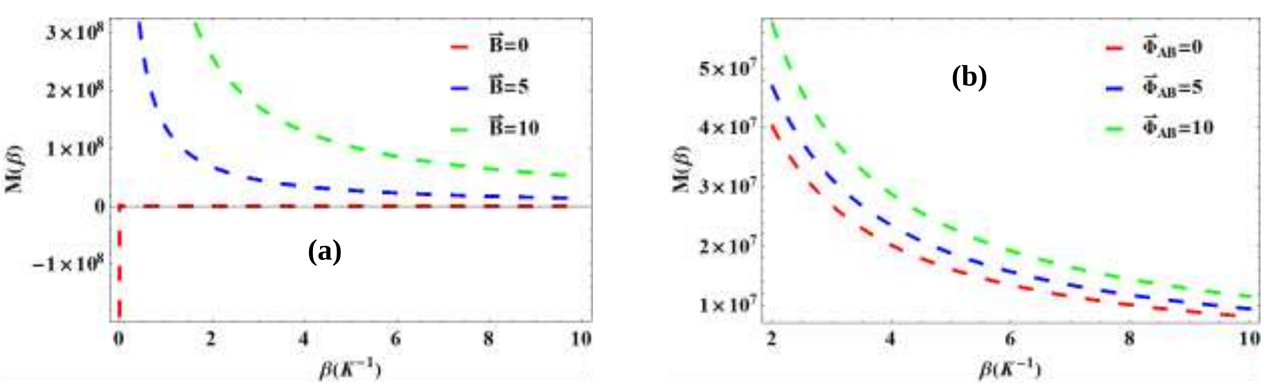

Figure 1. (a) Magnetization as a function of β varying with magnetic field, (b) Magnetization as a function of β varying with AB field.

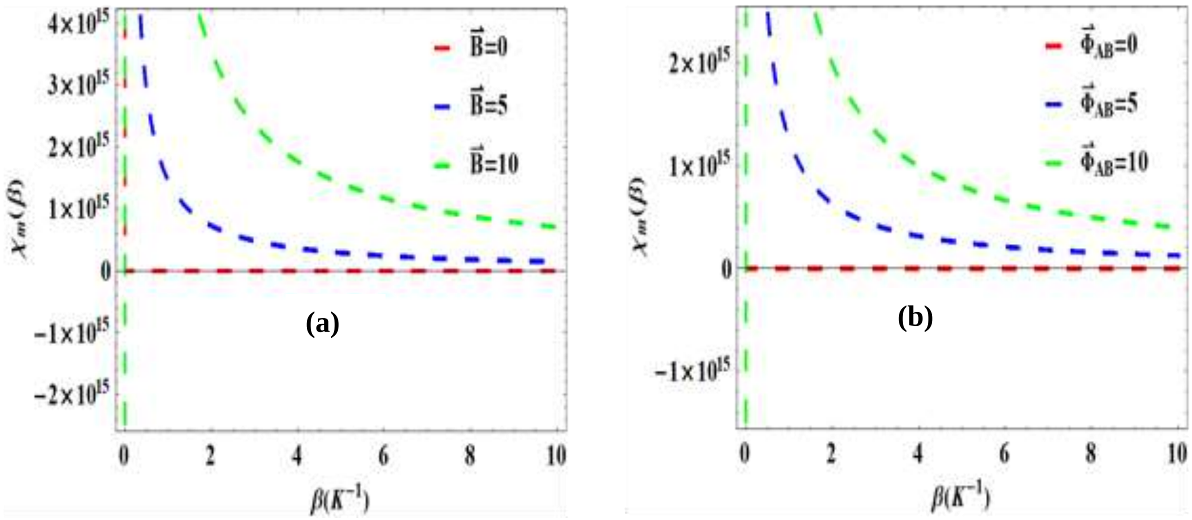

Figure 2. (a) Magnetic susceptibility as a function of β varying with magnetic field, (b) Magnetic susceptibility as a function of β varying with AB field.

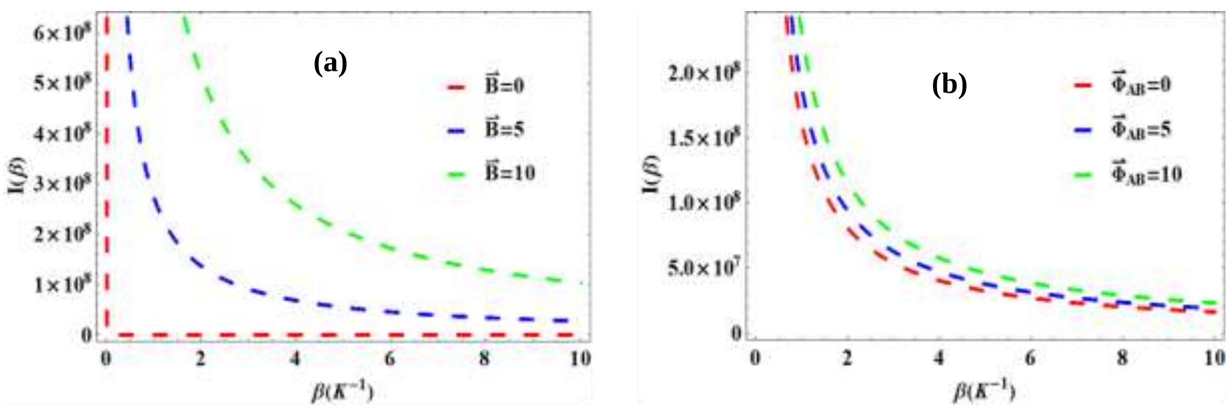

Figure 3. (a) Persistent current as a function of β varying with magnetic field, (b) Persistent current as a function of β varying with AB field.

DISCUSSION

The magnetization of the titanium carbide (TiC) diatomic molecule was analyzed as a function of inverse temperature $\beta = 1/(K_B T)$ under varying magnetic fields $\vec{B}$ and Aharonov–Bohm (AB) flux fields Φ_{AB}, as shown in Figure 1(a) and Figure 1(b), respectively. At zero magnetic field ($\vec{B} = 0$), the magnetization initially exhibits a sharp increase at very low temperatures and then remains nearly constant with further temperature increase. However, for stronger magnetic fields ($\vec{B} = 5$ and $\vec{B} = 10$), the magnetization decreases as temperature increases. Despite this decreasing trend, the overall magnitude of magnetization is higher for stronger magnetic fields. Similarly, in Figure 1(b), magnetization decreases with increasing temperature for AB flux values of $\Phi_{AB} = 0, 5$ and 10. As the AB flux increases, the overall magnetization also increases. This decrease in magnetization with rising temperature is attributed to enhanced thermal disorder, which disrupts the alignment of magnetic dipoles with the external magnetic field. These observations indicate that higher magnetic fields or AB flux values enhance overall magnetization, even as the thermal disorder reduces alignment at higher temperatures. A similar trend is observed in magnetic susceptibility (Figure 2(a) and Figure 2(b)) and persistent current (Figure 3(a) and Figure 3(b)), where both quantities decrease with increasing temperature under varying magnetic and AB flux fields. As the field strengths increase, the magnitudes of susceptibility and persistent current also increase. This behavior, characterized by a decrease with increasing temperature, is consistent with the findings reported by [32] for TiH diatomic molecules.

CONCLUSION

This study analyzed the magnetic properties of the TiC diatomic molecule under the combined influence of magnetic and Aharonov–Bohm flux fields using the generalized cosine Yukawa potential within the Nikiforov–Uvarov framework. The findings revealed that increasing the magnetic or AB flux field enhances the overall magnetization, magnetic susceptibility and persistent current, while rising temperature suppresses these quantities due to thermal disorder. These results highlight the significant role of magnetic and AB flux fields in controlling the quantum magnetic behavior of TiC.

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